

1,4-Benzoquinone
106-51-4 | DTXSID6020145

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.89e-01

Global applicability domain: Inside

Local applicability domain index: 5.52e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

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1,4-Benzoquinone

Measured: 0.2

Predicted: 4.89e-01

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2-Methyl-p-benzoquinone

Measured: 0.72

Predicted: 7.75e-01

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2,4,6-Cycloheptatrien-1-one, 3-hydroxy-

Measured: 0.81

Predicted: 1.06

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Salicylaldehyde

Measured: 1.81

Predicted: 1.45

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Benzaldehyde, 3-hydroxy-

Measured: 1.29

Predicted: 1.24